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Sensors Journal, IEEE , Volume: 3 , Issue: 4 , Aug. 2003

Pages:345 - 351

[\[Abstract\]](#) [\[PDF Full-Text \(614 KB\)\]](#) **IEEE JNL****2 A novel method of measuring the thickness of hydrated ultrathin polymer film by the force curve of atomic force microscopy***Wu, C.C.; Chang, H.C.;*

Microtechnologies in Medicine & Biology 2nd Annual International IEEE-EMB Special Topic Conference on , 2-4 May 2002

Pages:27 - 30

[\[Abstract\]](#) [\[PDF Full-Text \(436 KB\)\]](#) **IEEE CNF**

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Antennas and Propagation Society International Symposium, 2001. IEEE , Volume 3 , 8-13 July 2001

Pages:244 - 247 vol.3

[\[Abstract\]](#) [\[PDF Full-Text \(200 KB\)\]](#) IEEE CNF**2 Measurements of solder bump lifetime as a function of underfill material properties***Nysaether, J.B.; Lundstrom, P.; Liu, J.;*

The First IEEE International Symposium on Polymeric Electronics Packaging , 26-30 Oct. 1997

Pages:307 - 314

[\[Abstract\]](#) [\[PDF Full-Text \(640 KB\)\]](#) IEEE CNF**3 The effect of ring electrodes attachment to a corona gun on control of free ion concentration and back corona for improving powder paint appearance***Biris, A.S.; Mazumder, M.K.; Sims, R.A.; Yurteri, C.U.; Farmer, S.; Snodgrass, .*
Industry Applications, IEEE Transactions on , Volume: 39 , Issue: 6 , Nov.-Dec. 2003

Pages:1614 - 1621

[\[Abstract\]](#) [\[PDF Full-Text \(815 KB\)\]](#) IEEE JNL**4 Lensed plastic optical fiber employing concave end filled with high-index resin***Sakata, H.; Imada, A.;*

Lightwave Technology, Journal of , Volume: 20 , Issue: 4 , April 2002
Pages:638 - 642

[\[Abstract\]](#) [\[PDF Full-Text \(310 KB\)\]](#) [IEEE JNL](#)

5 Measurements of solder bump lifetime as a function of underfill material properties

Nysaether, J.B.; Lundstrom, P.; Liu, J.;

Components, Packaging, and Manufacturing Technology, Part A, IEEE Transactions on [see also Components, Hybrids, and Manufacturing Technology, IEEE Transactions on] , Volume: 21 , Issue: 2 , June 1998
Pages:281 - 287

[\[Abstract\]](#) [\[PDF Full-Text \(180 KB\)\]](#) [IEEE JNL](#)

6 Explosion model applied to an intense pulsed plasma source for thin film deposition

Pedrow, P.D.; Goyal, K.O.; Mabalingham, R.; Osman, M.A.;

Plasma Science, IEEE Transactions on , Volume: 25 , Issue: 1 , Feb. 1997
Pages:89 - 96

[\[Abstract\]](#) [\[PDF Full-Text \(216 KB\)\]](#) [IEEE JNL](#)

7 Compliant bumps for adhesive flip-chip assembly

Keswick, K.; German, R.L.; Breen, M.; Nolan, R.;

Components, Packaging, and Manufacturing Technology, Part B: Advanced Packaging, IEEE Transactions on [see also Components, Hybrids, and Manufacturing Technology, IEEE Transactions on] , Volume: 18 , Issue: 3 , Aug 1995
Pages:503 - 510

[\[Abstract\]](#) [\[PDF Full-Text \(752 KB\)\]](#) [IEEE JNL](#)

8 Polymeric cable terminators under accelerated aging in a fog chamber

Gorur, R.S.; Cherney, E.A.; Hackam, R.;

Power Delivery, IEEE Transactions on , Volume: 4 , Issue: 2 , April 1989
Pages:842 - 849

[\[Abstract\]](#) [\[PDF Full-Text \(828 KB\)\]](#) [IEEE JNL](#)

9 Effective indexing and filtering for similarity search in large biosequence databases

Ozturk, O.; Ferhatosmanoglu, H.;

Bioinformatics and Bioengineering, 2003. Proceedings. Third IEEE Symposium on , 10-12 March 2003
Pages:359 - 366

[\[Abstract\]](#) [\[PDF Full-Text \(844 KB\)\]](#) [IEEE CNF](#)

10 Augmenting SSEs with structural properties for rapid protein structure comparison

Chern-Hooi Chionh; Zhiyong Huang; Kian-Lee Tan; Zhen Yao;

Bioinformatics and Bioengineering, 2003. Proceedings. Third IEEE Symposium on , 10-12 March 2003
Pages:341 - 348

[\[Abstract\]](#) [\[PDF Full-Text \(401 KB\)\]](#) [IEEE CNF](#)

11 Nodal distance algorithm: calculating a phylogenetic tree comparison metric

Bluis, J.; Shin, D.G.;

Bioinformatics and Bioengineering, 2003. Proceedings. Third IEEE Symposium on , 10-12 March 2003

Pages:87 - 94

[\[Abstract\]](#) [\[PDF Full-Text \(333 KB\)\]](#) [IEEE CNF](#)

12 Estimation of the platelet glycoprotein (GP) Ib - von Willebrand factor (vWf) bond lifetime under hydrodynamic flow

Anand Kumar, R.; Jing-fei Dong; Lopez, J.A.; Cruz, M.A.; McIntire, L.V.;

[Engineering in Medicine and Biology, 2002. 24th Annual Conference and the Annual Fall Meeting of the Biomedical Engineering Society] EMBS/BMES Conference, 2002. Proceedings of the Second Joint , Volume: 1 , 2002

Pages:347 - 348 vol.1

[\[Abstract\]](#) [\[PDF Full-Text \(238 KB\)\]](#) [IEEE CNF](#)

13 Thermochromic behavior in novel conducting polymers at the solid-liquid phase transition

Onoda, M.; Tada, K.;

Dielectric Liquids, 2002. ICDL 2002. Proceedings of 2002 IEEE 14th International Conference on , 7-12 July 2002

Pages:373 - 376

[\[Abstract\]](#) [\[PDF Full-Text \(360 KB\)\]](#) [IEEE CNF](#)

14 A study of image retrieval by anchoring

Natsev, A.; Smith, J.R.;

Multimedia and Expo, 2002. ICME '02. Proceedings. 2002 IEEE International Conference on , Volume: 2 , 26-29 Aug. 2002

Pages:421 - 424 vol.2

[\[Abstract\]](#) [\[PDF Full-Text \(542 KB\)\]](#) [IEEE CNF](#)

15 A novel method of measuring the thickness of hydrated ultrathin polymer film by the force curve of atomic force microscopy

Wu, C.C.; Chang, H.C.;

Microtechnologies in Medicine & Biology 2nd Annual International IEEE-EMB Special Topic Conference on , 2-4 May 2002

Pages:27 - 30

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Engineering in Medicine and Biology Society, 2001. Proceedings of the 23rd Annual International Conference of the IEEE, Volume: 1, 25-28 Oct. 2001

Pages:733 - 736 vol.1

[\[Abstract\]](#) [\[PDF Full-Text \(548 KB\)\]](#) IEEE CNF17 **Effect of intermolecular interactions on charge transport and light-emission in organic light emitting diodes***Lupton, J.M.; Samuel, I.D.W.; Beavington, R.; Burn, P.L.; Bassler, H.;*

Lasers and Electro-Optics Europe, 2000. Conference Digest. 2000 Conference on , 10-15 Sept 2000

Pages:1 pp.

[\[Abstract\]](#) [\[PDF Full-Text \(84 KB\)\]](#) IEEE CNF18 **Computer biochemistry and molecular technology of the underwater biosensor creation: study of the natural chemical substance population***Zamyatnin, A.A.;*

Underwater Technology, 2000. UT 00. Proceedings of the 2000 International Symposium on , 23-26 May 2000

Pages:451 - 456

[\[Abstract\]](#) [\[PDF Full-Text \(412 KB\)\]](#) IEEE CNF19 **A new linguistic fuzzy approach to recognition of olfactory signals***Lazzerini, B.; Maggiore, A.; Marcelloni, F.;*

Neural Networks, 1999. IJCNN '99. International Joint Conference on , Volume: , 10-16 July 1999

Pages:3225 - 3229 vol.5

[\[Abstract\]](#) [\[PDF Full-Text \(456 KB\)\]](#) [IEEE CNF](#)

20 Fractals for hybrid orbitals in protein models

Torrens, F.; Sanchez-Marin, J.; Nebot-Gil, I.;

Information Technology Applications in Biomedicine, 1998. ITAB 98. Proceeding 1998 IEEE International Conference on , 16-17 May 1998

Pages:45 - 50

[\[Abstract\]](#) [\[PDF Full-Text \(272 KB\)\]](#) [IEEE CNF](#)

21 Experimental and numerical study of underfill encapsulation of flip-chips using conductive epoxy polymer bumps

Ni, G.; Gordon, M.H.; Schmidt, W.F.; Muyshondt, A.;

Electronic Components and Technology Conference, 1997. Proceedings., 47th , 18-21 May 1997

Pages:859 - 865

[\[Abstract\]](#) [\[PDF Full-Text \(560 KB\)\]](#) [IEEE CNF](#)

22 Basic investigations of the performance of droplets on electrically stressed polymer surfaces

Kloes, H.-J.; Koenig, D.;

Electrical Insulation and Dielectric Phenomena, 1997. IEEE 1997 Annual Report. Conference on , Volume: 2 , 19-22 Oct. 1997

Pages:374 - 377 vol.2

[\[Abstract\]](#) [\[PDF Full-Text \(504 KB\)\]](#) [IEEE CNF](#)

23 New hashing techniques and their application to a protein structure database system

Akutsu, T.; Onizuka, K.; Ishikawa, M.;

System Sciences, 1995. Vol. V. Proceedings of the Twenty-Eighth Hawaii International Conference on , Volume: 5 , 3-6 Jan. 1995

Pages:197 - 206 vol.5

[\[Abstract\]](#) [\[PDF Full-Text \(640 KB\)\]](#) [IEEE CNF](#)

24 Breakdown voltages of dielectric-coated sphere-plane electrode configurations in high vacuum

Konig, D.; Heinemeyer, R.; Scherb, V.;

Electrical Insulation, 1988., Conference Record of the 1988 IEEE International Symposium on , 5-8 June 1988

Pages:60 - 63

[\[Abstract\]](#) [\[PDF Full-Text \(292 KB\)\]](#) [IEEE CNF](#)

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1 Fast detection of common geometric substructure in proteins

L. Paul Chew, Dan Huttenlocher, Klara Kedem, Jon Kleinberg

April 1999 Proceedings of the third annual international conference on Computationa

Full text available: pdf(1.18 MB)

Additional Information: full citation, references, index terms

2 Detection of three-dimensional patterns of atoms in chemical structures

Arthur M. Lesk

April 1979

Communications of the ACM, Volume 22 Issue 4

Full text available: pdf(599.69 KB)

Additional Information: full citation, abstract, refer

An algorithm for detecting occurrences of a three-dimensional pattern of objects. The search technique presented uses the geometric structure of the pattern to c candidates for matching. This is useful in cases where the properties of each atc adequately limit the number of sets of possible matchings. Several applications are: (1) i ...

Keywords: chemical structure search, crystal-structure analysis, drug analysis a three-dimensional pattern recognition

3 Hybrid genetic algorithms for polypeptide energy minimization

Laurence D. Merkle, Robert L. Gaulke, Gary B. Lamont, George H. Gates, Ruth Pac
February 1996 Proceedings of the 1996 ACM symposium on Applied Computir


Full text available:  pdf(689.75 KB)

Additional Information: full citation, references, citing

Keywords: Baldwinian evolution, conjugate gradient, genetic algorithms, probab
folding

4 Keynote address: Visualization challenges for a new cyberpharmaceutical (

Russell J. Turner, Kabir Chaturvedi, Nathan J. Edwards, Daniel Fasulo, Aaron L. Ha
Jason R. Miller, Knut Reinert, Karin A. Remington, Russell Schwartz, Brian Walenz,
October 2001 Proceedings of the IEEE 2001 symposium on parallel and large-data

Full text available:  pdf(3.07 MB)

Additional Information: full citation, abstract, reference

In recent years, an explosion in data has been profoundly changing the field of t
areas of expertise, particularly in the handling of data. One vital area that has s
to communicate the large quantities of diverse and complex information that is l
a number of visualization problems in the course of developing tools for bioinfor
data generation ...

5 Polypeptide structure prediction: real-value versus binary hybrid genetic alg

Charles E. Kaiser, Gary B. Lamont, Laurence D. Merkle, George H. Gates, Ruth Pac
April 1997 Proceedings of the 1997 ACM symposium on Applied computing

Full text available:  pdf(727.53 KB)

Additional Information: full citation, references, citing

Keywords: genetic algorithms, hybrid genetic algorithms, polypeptide structure
genetic algorithms

6 The threading approach to the inverse protein folding problem

Temple F. Smith, Loredana Lo Conte, Jadwiga Bienkowska, Bob Rogers, Chrysanth
January 1997 Proceedings of the first annual international conference on Computati

Full text available:  pdf(680.95 KB)

Additional Information: full citation, references, citings, inc

7 Coupled optimization in protein docking

Julie C. Mitchell, J. Ben Rosen, Andrew T. Phillips, Lynn F. Ten Eyck

April 1999 Proceedings of the third annual international conference on Computational

Full text available:  pdf(702.99 KB)

Additional Information: full citation, references, index term

8 Interactive computer graphics and macromolecular structures

Peter J. Bond

March 1972 ACM SIGGRAPH Computer Graphics , Proceedings of the 1972 SIGGRAPH
medicine, Volume 6 Issue 4

Full text available:  pdf(935.08 KB)

Additional Information: full citation, abstract, referen

In 1964 on Project MAC at MIT, Levinthal and Langridge first applied interactive building (1, 2). Since then a number of laboratories have developed computer g needs (3, 4, 5, 6). I shall begin by describing the system that we have develop Graphics Laboratory during the past year to investigate macromolecular structu

9 Minimizing the Lennard-Jones potential function on a massively parallel co

G. L. Xue, R. S. Maier, J. B. Rosen

August 1992 Proceedings of the 6th international conference on Supercomputi

Full text available:  pdf(636.32 KB)

Additional Information: full citation, abstract, references, c

The Lennard-Jones potential energy function arises in the study of low-energy s cluster statics. This paper presents a mathematical treatment of the potential fu function of the cluster size, in both two and three dimensional configurations. Th minimization of a linear chain, or polymer, in two-dimensional space to illustrate cluster size. An algorithm is ...

10 Large scale molecular dynamics simulations with fast multipole implementa

Zhiqiang Wang, James A. Lupo, Alan M. McKenney, Ruth Pachter

January 1999 Proceedings of the 1999 ACM/IEEE conference on Supercomputing (CI


Full text available:  pdf(748.81 KB)

Additional Information: full citation, references, citings, index terms

11 Simulation and preferences: Virtual spring manipulators for particle steering responsive workbench

Michal Koutek, Jeroen van Hees, Frits H. Post, A. F. Bakker

May 2002 Proceedings of the workshop on Virtual environments 2002

Full text available:  pdf(6.52 MB)

Additional Information: full citation, abstract, referenc

In this paper we present new virtual spring manipulator-based tools for steering simulations in virtual environments. We briefly overview the MolDRIVE system, steering environment for molecular dynamics real-time simulations, which is the implementation. Our study concentrates on visual feedback tools. We compare a with two other methods using a spring mani ...

12 Approximation of protein structure for fast similarity measures

Fabian Schwarzer, Itay Lotan

April 2003 Proceedings of the seventh annual international conference on Computa

Full text available:  pdf(212.43 KB)

Additional Information: full citation, abstract, referen

It is shown that structural similarity between proteins can be decided well with r common similarity measures. The full C? representation contains redundant info topology of proteins and a limit on their compactness due to excluded volume. / proteins justifies approximating subchains by their centers of mass. For not too and ...

Keywords: approximation of structure, nearest-neighbor search, protein structu

13 SIGSAM BULLETIN: Computer algebra in the life sciences

Michael P. Barnett

December 2002

ACM SIGSAM Bulletin, Volume 36 Issue 4

Full text available:  pdf(240.15 KB)

Additional Information: full citation, abstract,

This note (1) provides references to recent work that applies computer algebra literature that explains the biological background of each application, (3) states (4) mentions the benefits of CA, and (5) suggests some topics for future work.

14 Extracting structural information using time-frequency analysis of protein NI

Christopher James Langmead, Bruce Randall Donald

April 2001 Proceedings of the fifth annual international conference on Computati

Full text available:  pdf(623.73 KB)


Additional Information: full citation, abstract, referen

High-throughput, data-directed computational protocols for *Stru* are required in order to evaluate the protein products of genes f comparable to current gene-sequencing technology. To develop are required that can quickly extract significantly more structural experimental data. This paper presents a new class of signal prc magnetic re ...

15 GRAMPS - A graphics language interpreter for real-time, interactive, three-animation

T. J. O'Donnell, Arthur J. Olson

August 1981 ACM SIGGRAPH Computer Graphics , Proceedings of the 8th annual computer graphics conference on interactive techniques, Volume 15 Issue 3

Full text available:  pdf(1.19 MB)

Additional Information: full citation, abstract, references, comments

GRAMPS, a graphics language interpreter has been developed in FORTRAN 77 to interface with a real-time interactive vector display list processor (Evans and Sutherland Multi-Picture-System). The language make it very useful and convenient for real-time scene construction, and the language syntax allows natural interaction with scene elements as well as easy integration with graphics devices. GRAMPS facilitates the ...

Keywords: Graphics language interpreter, Picture editor, Real-time animation, Visual programming

16 Molecular simulation of rheological properties using massively parallel supercomputing

R. K. Bhupathiraju, S. T. Cui, S. Gupta, H. D. Cochran, P. T. Cummings

November 1996 Proceedings of the 1996 ACM/IEEE conference on Supercomputing

Full text available:  pdf(120.44 KB)

Additional Information: full citation, abstract, references, comments

Advances in parallel supercomputing now make possible molecular-based engineering simulations. These simulations soon revolutionize many technologies, such as those involving polymers and thin films. We have developed a suite of message-passing codes for classical molecular simulation of crystalline and amorphous materials and have completed a number of demonstration calculations. The technological importance with each (describe ...)

17 Using motion planning to map protein folding landscapes and analyze folding

Nancy M. Amato, Ken A. Dill, Guang Song

April 2002 Proceedings of the sixth annual international conference on Computational Molecular Biology

Full text available:  pdf(4.00 MB)

Additional Information: full citation, abstract, references, comments

We present a novel approach for studying the kinetics of protein folding. The framework uses motion planning techniques called *probabilistic roadmap* methods (prms) that have been successful in many applications. In our previous work, we used a Prm-based technique to study protein folding and obtained encouraging results. In this paper, we describe how our motion planning approach can be used to study protein folding ...

18 Protein structure determination using protein threading and sparse NMR data

Ying Xu, Dong Xu, Oakley H. Crawford, J. Ralph Einstein, Engin Serpersu

April 2000 Proceedings of the fourth annual international conference on Computational Biology

Full text available:  pdf(663.42 KB)

Additional Information: full citation, abstract, references

It is well known that the NMR method for protein structure determination is only effective for small proteins and that its effectiveness decreases very rapidly as the protein size goes beyond about 30 kD. We have recently developed a method for protein structure determination that can fully utilize partial NMR data as calculation constraints. Our new protein threading algorithm that guarantees to find a globally optimal protein sequence and a template structure, ...

Keywords: NMR, energy minimization, fold recognition, protein structure prediction, protein threading

19 Architectural requirements of parallel scientific applications with explicit communication

R. Cypher, A. Ho, S. Konstantinidou, P. Messina

May 1993 ACM SIGARCH Computer Architecture News , Proceedings of the 20th annual SIGARCH/Computer architecture, Volume 21 Issue 2

Full text available:  pdf(1.29 MB)

Additional Information: full citation, abstract, references, comments

This paper studies the behavior of scientific applications running on distributed architectures. We quantify the floating point, memory, I/O and communication requirements of high performance explicit communication. In addition to quantifying these requirements for various processors, we develop analytical models for the effects of changing the problem size and the number of processors of the ...

20 Assessment of ab initio protein structure prediction

Arthur M. Lesk

March 1998 Proceedings of the second annual international conference on Computational Biology

Full text available:  pdf(945.12 KB)

Additional Information: full citation, references, index terms

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21 De Novo peptide sequencing via tandem mass spectrometry: a graph-theor

Vlado Dan?ík, Theresa A. Addona, Karl R. Clauser, James E. Vath

April 1999 Proceedings of the third annual international conference on Computat

Full text available: pdf(1.24 MB)

Additional Information: full citation, references, citings, index ter

22 Regression analysis of multiple protein structures

Thomas D. Wu, Trevor Hastie, Scott C. Schmidler, Douglas L. Brutlag

March 1998 Proceedings of the second annual international conference on Computat

Full text available: pdf(1.04 MB)

Additional Information: full citation, references, index term

23 Finding the consensus shape for a protein family

L. Paul Chew, Klara Kedem

June 2002 Proceedings of the eighteenth annual symposium on Computational Geometry

Full text available:  pdf(211.67 KB)

Additional Information: full citation, abstract, references

We define and prove properties of the *consensus shape for a family of proteins*, a compact summary of the significant structural information for a protein family. It is a geometric relationship between corresponding alpha carbons then that relations. In particular, distances and angles that are consistent across family members are the spacings ...

Keywords: dynamic programming, multiple alignment, protein alignment, protein RMS

24 The NOESY jigsaw: automated protein secondary structure and main-chain NMR data

Chris Bailey-Kellogg, Alik Widge, John J. Kelley, Marcelo J. Berardi, John H. Bushweller
April 2000 Proceedings of the fourth annual international conference on Computational Molecular Biology

Full text available:  pdf(907.80 KB)

Additional Information: full citation, abstract, references

High-throughput, data-directed computational protocols for *Stru* are required in order to evaluate the protein products of genes of a scale comparable to current gene-sequencing technology. This paper presents a novel high-throughput, automated approach to protein structure determination by nuclear magnetic resonance (NMR). JIGSAW applies graph algorithms and other techniques, and ...

25 The hierarchical organization of molecular structure computations

Cheng Che Chen, Jaswinder Pal Singh, Russ B. Altman

March 1998 Proceedings of the second annual international conference on Computational Molecular Biology

Full text available:  pdf(992.98 KB)

Additional Information: full citation, references, index terms

26 Algorithmic determination of core positions in the VL and VH domains of immunoglobulin

Israel Gelfand, Alexander Kister, Casimir Kulikowski, Ognian Stoyanov

March 1998 Proceedings of the second annual international conference on Computational Molecular Biology

Full text available:  pdf(962.19 KB)

Additional Information: full citation, references, index terms

27 Trilogy: discovery of sequence-structure patterns across diverse proteins

Phil Bradley, Peter S. Kim, Bonnie Berger

April 2002 Proceedings of the sixth annual international conference on Computati

Full text available:  pdf(3.86 MB)

Additional Information: full citation, abstract, references

We describe a new computer program, Trilogy, for the automated discovery of s
Trilogy implements a pattern discovery algorithm that begins with an exhaustive
patterns; a subset of these patterns are selected as seeds for an extension proc
identified. A key feature of the method is explicit treatment of both the sequenc
motifs: each Trilogy pattern is a pair ...

28 Massively parallel simulations of diffusion in dense polymeric structures

Jean-Loup Faulon, J. David Hobbs, David M. Ford, Robert T. Wilcox

November 1997 Proceedings of the 1997 ACM/IEEE conference on Supercomput

Full text available:  pdf(92.74 KB)

Additional Information: full citation, abstract,

An original computational technique to generate close-to-equilibrium dense poly
small gases are studied on the equilibrated structures using massively parallel n
the Intel Teraflops (9216 Pentium Pro processors) and Intel Paragon (1840 proc
state-of-the-art equilibration methods this new technique appears to be faster b
advantage of the technique i ...

Keywords: gas diffusion, molecular builder, molecular dynamics, polymer, terafl

29 Determining contact energy function for continuous state models of globula

Y. Zenmei Ohkubo, Gordon M. Crippen

April 2000 Proceedings of the fourth annual international conference on Computati

Full text available:  pdf(698.70 KB)

Additional Information: full citation, abstract,

One of the approaches to protein structure prediction is to obtain
recognize the native conformation of a given sequence among a
discriminations can be done by assigning the lowest energy to th
guarantee that the native is in the zoo. Well-adjusted functions,
for other (near-) natives. Here the aim is the discrimination at r
difference between the ...

30 A solvation potential with improved contact definitions and optimized by ext

Alan A. Dombkowski, Gordon M. Crippen

April 1999 Proceedings of the third annual international conference on Computations

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31 A framework for improving protein structure predictions by teamwork

Luigi Palopoli, Giorgio Terracina

January 2003 Proceedings of the First Asia-Pacific bioinformatics conference on Bio

Full text available:  pdf(306.78 KB)

Additional Information: full citation, abstract, referenc

Predicting the three dimensional structure of proteins is a difficult task. In the last years, a growing number of protein structure prediction tools is becoming available, some of which either address some aspects of the predictions or on some categories of proteins. In this paper, we propose a framework for performing this task taking into account different protein chemical representations. The framework applies different pr ...

Keywords: collaborative computation, heterogeneous representations, multi-agent

32 Session 19: biomedical applications: Parallel protein structure determination

Cheng Che Chen, Jaswinder Pal Singh, William B. Poland, Russ B. Altman

November 1994 Proceedings of the 1994 ACM/IEEE conference on Supercomputing

Full text available:  pdf(957.79 KB)


Additional Information: full citation, abstract, r

Molecular structure determination is an important task in biology because of the function of biological molecules. Individual sources of information about molecular structure are not sufficiently abundant to define the structure to high accuracy by the probabilistic algorithm, PROTEAN, which can incorporate multiple sources of uncertainty. We describe a method for determining the three-dimensional structure of molecules and al ...

33 An algorithm with linear complexity for interactive, physically-based modeling

Mark C. Surles

July 1992 ACM SIGGRAPH Computer Graphics, Proceedings of the 19th annual conference on interactive techniques, Volume 26 Issue 2

Full text available:  pdf(1.76 MB)

Additional Information: full citation, references, citing:

Keywords: Lagrange multiplier method, constrained systems, molecular modeling

34 The principled design of large-scale recursive neural network architectures for the protein structure prediction problem

Pierre Baldi, Gianluca Pollastri

December 2003 The Journal of Machine Learning Research, Volume 4

Full text available:  pdf(231.40 KB)

Additional Information: full citation

We describe a general methodology for the design of large-scale recursive neural networks for the protein structure prediction problem, which comprises three fundamental steps: (1) representation of a given domain (DAGs) to connect visible and hidden node variables; (2) parameterization of the DAGs by feedforward neural networks; and (3) application of weighted DAG connections to capture s ...

Miquel L. Teodoro, George N. Phillips, Lydia E. Kavraki

April 2002

Proceedings of the sixth annual international conference on Computat

Full text available: pdf(2.03 MB)

Additional Information: full citation, abstract, reference

Proteins are involved either directly or indirectly in all biological processes in living organisms. It is well known that conformational changes of proteins can critically affect their ability to bind to other molecules. Therefore, modeling protein motion and flexibility will contribute to the understanding of key biological processes. However, protein flexibility has proven a very difficult task. Experimental laboratory methods

...

Cheng Che Chen, Jaswinder Pal Singh, Russ B. Altman

November 1996

Proceedings of the 1996 ACM/IEEE conference on Supercomput

Full text available: pdf(220.93 KB)

Additional Information: full citation, abstract, references, c

Determining the structure of biological macromolecules such as proteins and nucleic acids is a central goal of molecular biology because of the intimate relation between form and function of these molecules. Unfortunately, the data about molecular structure are subject to varying degrees of uncertainty. This paper describes the parallelization of a probabilistic algorithm for combining multiple sources of uncertain data to determine the three-dimensional structure of molecule ...

Hans-Peter Lenhof

January 1997

Proceedings of the first annual international conference on Computatic

Full text available: pdf(1.30 MB)

Additional Information: full citation, references, citings, index te

Sangeeta Sawant, A. S. Kolaskar

January 2003

Proceedings of the First Asia-Pacific bioinformatics conference on Bio

Full text available: pdf(1.53 MB)

Additional Information: full citation, abstract, reference

A strategy using multiple runs of MD simulations has been used for conformational sampling to demonstrate the effectiveness of the strategy to sample the conformational space of a protein in a single MD simulation. Further, the use of cluster analysis and C α -C α distances has been employed to identify conformations of the peptide that are generated in the relatively short time scale simulations.

Keywords: cluster analysis, conformational searches, multiple MD simulations, o

39 A unified sequence-structure classification of protein sequences: combining the protein space

Golan Yona, Michael Levitt

April 2000 Proceedings of the fourth annual international conference on Computati

Full text available:  pdf(952.18 KB)

Additional Information: full citation, abstract

We analyze all known protein sequences in search for a global n consistent in terms of both sequence and structure. Our goal is t protein domains, beyond those detected by sequence-based me three-dimensional (3D) model for each of the sequences that ar known 3D structure. This analysis uses both sequence and struc of all protein sequences in a ...

40 Structural alignment of large—size proteins via lagrangian relaxation

Alberto Caprara, Giuseppe Lancia

April 2002 Proceedings of the sixth annual international conference on Computat

Full text available:  pdf(1.65 MB)

Additional Information: full citation, abstract, reference

We illustrate a new approach to the Contact Map Overlap problem for the comp is based on formulating the problem as an integer linear program and then rela constraints. This relaxation is solved by computing a sequence of simple alignme near--optimal Lagrangian multipliers are found by subgradient optimization. By speedup over the best ...

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21 De Novo peptide sequencing via tandem mass spectrometry: a graph-theoretic approach
Vlado Dan?ik, Theresa A. Addona, Karl R. Clauser, James E. Vath
April 1999 Proceedings of the third annual international conference on Computational Biology
Full text available: pdf(1.24 MB) Additional Information: full citation, references, citings, index term

22 Regression analysis of multiple protein structures
Thomas D. Wu, Trevor Hastie, Scott C. Schmidler, Douglas L. Brutlag
March 1998 Proceedings of the second annual international conference on Computational Biology
Full text available: pdf(1.04 MB) Additional Information: full citation, references, index term

23 Finding the consensus shape for a protein family

L. Paul Chew, Klara Kedem

June 2002 Proceedings of the eighteenth annual symposium on Computational Geometry

Full text available:  pdf(211.67 KB)

Additional Information: full citation, abstract, references

We define and prove properties of the *consensus shape for a family of proteins*, compact summary of the significant structural information for a protein family. It is a geometric relationship between corresponding alpha carbons then that relations. In particular, distances and angles that are consistent across family members are the spacings ...

Keywords: dynamic programming, multiple alignment, protein alignment, protein RMS

24 The NOESY jigsaw: automated protein secondary structure and main-chain NMR data

Chris Bailey-Kellogg, Alik Widge, John J. Kelley, Marcelo J. Berardi, John H. Bushwiler
 April 2000 Proceedings of the fourth annual international conference on Computational Biology

Full text available:  pdf(907.80 KB)

Additional Information: full citation, abstract, references

High-throughput, data-directed computational protocols for *Structure* are required in order to evaluate the protein products of genes for which data is comparable to current gene-sequencing technology. This paper presents a novel high-throughput, automated approach to protein structure determination by nuclear magnetic resonance (NMR). JIGSAW applies graph algorithms and dynamic programming techniques, and ...

25 The hierarchical organization of molecular structure computations

Cheng Che Chen, Jaswinder Pal Singh, Russ B. Altman

March 1998 Proceedings of the second annual international conference on Computational Biology

Full text available:  pdf(992.98 KB)

Additional Information: full citation, references, index terms

26 Algorithmic determination of core positions in the VL and VH domains of immunoglobulins

Israel Gelfand, Alexander Kister, Casimir Kulikowski, Ognyan Stoyanov

March 1998 Proceedings of the second annual international conference on Computational Biology

Full text available:  pdf(962.19 KB)

Additional Information: full citation, references, index terms

31 A framework for improving protein structure predictions by teamwork

Luigi Palopoli, Giorgio Terracina

January 2003 Proceedings of the First Asia-Pacific bioinformatics conference on Bioinformatics

Full text available:  pdf(306.78 KB)

Additional Information: full citation, abstract, references

Predicting the three dimensional structure of proteins is a difficult task. In the last years, a number of tools have been proposed for performing this task taking into account different protein chemical features. A growing number of protein structure prediction tools is becoming available, some of which either improve some aspects of the predictions or on some categories of proteins. In this paper, we propose a framework for applying different pr ...

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32 Session 19: biomedical applications: Parallel protein structure determination

Cheng Che Chen, Jaswinder Pal Singh, William B. Poland, Russ B. Altman

November 1994 Proceedings of the 1994 ACM/IEEE conference on Supercomputing

Full text available:  pdf(957.79 KB)

Additional Information: full citation, abstract, references

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Mark C. Surles

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Pierre Baldi, Gianluca Pollastri

December 2003 The Journal of Machine Learning Research, Volume 4

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Additional Information: full citation

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35 A dimensionality reduction approach to modeling protein flexibility

Miguel L. Teodoro, George N. Phillips, Lydia E. Kavraki

April 2002 Proceedings of the sixth annual international conference on Computat

Full text available:  pdf(2.03 MB)

Additional Information: full citation, abstract, reference

Proteins are involved either directly or indirectly in all biological processes in livi that conformational changes of proteins can critically affect their ability to bind c modeling protein motion and flexibility will contribute to the understanding of ke protein flexibility has proven a very difficult task. Experimental laboratory methc

...

36 Parallel hierarchical molecular structure estimation

Cheng Che Chen, Jaswinder Pal Singh, Russ B. Altman

November 1996 Proceedings of the 1996 ACM/IEEE conference on Supercomput

Full text available:  pdf(220.93 KB)


Additional Information: full citation, abstract, references, c

Determining the structure of biological macromolecules such as proteins and nu molecular biology because of the intimate relation between form and function of data about molecular structure are subject to varying degrees of uncertainty. Pr parallelization of a probabilistic algorithm for combining multiple sources of unce three-dimensional structure of molecule ...

37 New contact measures for the protein docking problem

Hans-Peter Lenhof

January 1997 Proceedings of the first annual international conference on Computatic


Full text available:  pdf(1.30 MB)

Additional Information: full citation, references, citings, index te

38 Multiple molecular dynamics simulations of a 28mer oligopeptide reveal enl space

Sangeeta Sawant, A. S. Kolaskar

January 2003 Proceedings of the First Asia-Pacific bioinformatics conference on Bioi

Full text available:  pdf(1.53 MB)

Additional Information: full citation, abstract, reference

A strategy using multiple runs of MD simulations has been used for conformation demonstrate the effectiveness of the strategy to sample the conformational spa MD simulation. Further, the use of cluster analysis and C? distances has been m peptide that are generated in the relatively short time scale simulations.

Keywords: cluster analysis, conformational searches, multiple MD simulations, o

39 A unified sequence-structure classification of protein sequences: combining the protein space

Golan Yona, Michael Levitt

April 2000 Proceedings of the fourth annual international conference on Computati

Full text available:  pdf(952.18 KB)

Additional Information: full citation, abstract

We analyze all known protein sequences in search for a global n consistent in terms of both sequence and structure. Our goal is f protein domains, beyond those detected by sequence-based me three-dimensional (3D) model for each of the sequences that ar known 3D structure. This analysis uses both sequence and struc of all protein sequences in a ...

40 Structural alignment of large—size proteins via lagrangian relaxation

Alberto Caprara, Giuseppe Lancia

April 2002 Proceedings of the sixth annual international conference on Computat

Full text available:  pdf(1.65 MB)

Additional Information: full citation, abstract, reference

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41 Accurate performance evaluation, modelling and prediction of a message p middleware

Michela Taufer, Thomas Stricker

November 1998

Proceedings of the 1998 ACM/IEEE conference on Supercomput

Full text available: html(85.30 KB)

Additional Information: full citation, abstract, refe

In distributed and vectorized computing there is a large number of highly differ
application could run on. Therefore most traditional parallel codes are ill equippe
usage or their behavior at run time and the corresponding data are rarely publis
of an application and its platform systematically. As an improvement over the cl
integrated approach to pe ...

Keywords: PVM, application design methods, computer architecture, molecular c
middleware, performance monitoring, scientific application codes

42 Chain growth algorithms for HP-type lattice proteins

Erich Bornberg-Bauer

January 1997

Proceedings of the first annual international conference on Computatic

Full text available: pdf(1.13 MB)

Additional Information: full citation, references, citings, index f

Keywords: chain growth algorithm, cotranslational foldability, lattice models, loc

43 Interactive modeling enhanced with constraints and physics with application

Mark C. Surles

June 1992

Proceedings of the 1992 symposium on Interactive 3D graphics

Full text available:  pdf(1.03 MB)

Additional Information: full citation, references, citings, index

44 Comprehensive statistical method for protein fold recognition

Jadwiga R. Biełkowska, Lihua Yu, Sophia Zarakovich, Robert G. Rogers, Temple I

April 2000

Proceedings of the fourth annual international conference on Computati

Full text available:  pdf(1.08 MB)

Additional Information: full citation, abstract, r


We present a protein fold recognition method that uses a compr of structural Hidden Markov Models (HMMs). The structure/fold i the probabilities of all sequence-to-structure alignments Conven dictate that the optimal alignment can give an estimate of the lc conformation imposed by the structural model. The alignment is that is interpret ...

45 Multi Relational Data Mining (MRDM): Multi-relational data mining: an intro

Sašo Džeroski

July 2003

ACM SIGKDD Explorations Newsletter, Volume 5 Issue 1

Full text available:  pdf(1.71 MB)

Additional Information: full citation, abstract, refere

Data mining algorithms look for patterns in data. While most existing data minir data table, multi-relational data mining (MRDM) approaches look for patterns th a relational database. In recent years, the most common types of patterns and i have been extended to the multi-relational case and MRDM now encompasses r discovery, MR decision tree ...


Keywords: inductive logic programming, multi-relational data mining, relational relational decision trees, relational distance-based methods

46 RAPID: randomized pharmacophore identification for drug design

P. W. Finn, L. E. Kavraki, J.-C. Latombe, R. Motwani, C. Shelton, S. Venkatasubrar

August 1997

Proceedings of the thirteenth annual symposium on Computational ge

Full text available:  pdf(1.28 MB)

Additional Information: full citation, references, citings, index terms

47 A new method for modeling and solving the protein fold recognition problem

Ying Xu, Dong Xu, Edward C. Uberbacher

March 1998 Proceedings of the second annual international conference on Computat

Full text available:  pdf(893.53 KB)

Additional Information: full citation, references, citings, index

48 ARIADNE: pattern-directed inference and hierarchical abstraction in proteir

Richard H. Lathrop, Teresa A. Webster, Temple F. Smith

November 1987

Communications of the ACM, Volume 30 Issue 11

Full text available:  pdf(1.30 MB)



Additional Information: full citation, abstract, references, citing:

The macro-molecular structural conformations of proteins exhibit higher order r complicated by many factors. ARIADNE searches for similarities between structu structure at levels more abstract than the primary sequence.

49 Computational approach to the statistical mechanics of protein folding

Ming-Hong Hao, Harold A. Scheraga

December 1995 Proceedings of the 1995 ACM/IEEE conference on Supercomputing (

Full text available:  pdf(5.92 MB)  html(2.06 KB)

Additional Information: full citation, references, index

50 A complete and effective move set for simplified protein folding

Neal Lesh, Michael Mitzenmacher, Sue Whitesides

April 2003 Proceedings of the seventh annual international conference on Computa

Full text available:  pdf(521.61 KB)

Additional Information: full citation, abstract, referenc

We present new lowest energy configurations for several large benchmark probl hydrophobic-hydrophilic model. We found these solutions with a generic implem apparently novel set of transformations that we call *pull moves*. Our experiment best solutions in 3 to 14 hours, on average. Pull moves appear quite effective ar search algorithms for the problem. Addit ...

Keywords: local moves, protein folding, tabu search

51 Session P8: nature visualization: Visualizing dynamic molecular conformati

Johannes Schmidt-Ehrenberg, Daniel Baum, Hans Christian Hege

October 2002

Proceedings of the conference on Visualization '02

Full text available:  pdf(2.72 MB)

Additional Information: full citation, abstract, references,

The bioactivity of a molecule strongly depends on its metastable conformational these. Therefore, conformation analysis and visualization is a basic prerequisite processes. We present techniques for visual analysis of metastable molecular cor applicable methods for alignment of molecular geometries, as well as methods f metastable conformations. All an ...


Keywords: drug design, molecular conformation analysis, molecular modeling, u

52 Stochastic roadmap simulation: an efficient representation and algorithm fo

Mehmet Serkan Apaydin, Douglas L. Brutlag, Carlos Guestrin, David Hsu, Jean-Cla

April 2002

Proceedings of the sixth annual international conference on Computati

Full text available:  pdf(2.03 MB)

Additional Information: full citation, abstract, references, cil

Classic techniques for simulating molecular motion, such as the Monte Carlo and individual motion pathways one at a time and spend most of their time trying to energy landscape of a molecule. Their high computational cost prevents them fr pathways. We introduce Stochastic Roadmap Sirmulation (SRS), a new approach motion by simultaneously examining multip ...

53 Multi Relational Data Mining (MRDM): Biological applications of multi-relati

David Page, Mark Craven

July 2003

ACM SIGKDD Explorations Newsletter, Volume 5 Issue 1

Full text available:  pdf(1.12 MB)

Additional Information: full citation, abstract, referer


Biological databases contain a wide variety of data types, often with rich relatio multi-relational data mining techniques frequently are applied to biological data. of multi-relational data mining to biological data, taking care to cover a broad ra techniques.

54 Efficient database screening for rational drug design using pharmacophore

Steven M. LaValle, Paul W. Finn, Lydia E. Kavrak, Jean-Claude Latombe

April 1999

Proceedings of the third annual international conference on Computatio

Full text available:  pdf(1.70 MB)

Additional Information: full citation, references, citings,

55 On approximating arbitrary metrics by tree metrics

Yair Bartal

May 1998 Proceedings of the thirtieth annual ACM symposium on Theory of computation

Full text available:  pdf(4.11 MB)

Additional Information: full citation, references, citations, index terms

56 Protein structure prediction by a data-level parallel algorithm

X. Zhang, D. Waltz, J. P. Mesirov

August 1989

Proceedings of the 1989 ACM/IEEE conference on Supercomputing

Full text available:  pdf(907.03 KB)

Additional Information: full citation, abstract, references

We have developed a software system, PHI-PSI, on the Connection Machine that uses information from a database of 112 known protein structures (selected from the Protein Data Bank) to predict the structures of other proteins. The ϕ and ψ angles of each amino acid (together with its immediate neighbors) in a protein are used to represent its 3-D structure.

57 Topology preserving dynamic load balancing for parallel molecular simulation

David F. Hegarty, M. T. Kechadi

November 1997

Proceedings of the 1997 ACM/IEEE conference on Supercomputing

Full text available:  pdf(227.39 KB)

Additional Information: full citation, abstract, references

Understanding the behavior of molecular systems such as DNA and proteins is a complex task. Most research laboratories now have a collection of heterogeneous parallel computers brought to bear on this problem - high end PCs, various different workstations, etc. [8, 11, 20]. Much work is currently being done on programming tools to exploit this work to date is aimed ...

58 Efficient algorithms for protein sequence design and the analysis of certain

Jon M. Kleinberg

April 1999

Proceedings of the third annual international conference on Computational Biology

Full text available:  pdf(1.52 MB)

Additional Information: full citation, references, citations, index terms

59 Prediction of 3D structure of envelope glycoprotein of Sri Lanka strain of Japanese encephalitis virus

Urmila Kulkarni-Kale, A. S. Kolaskar

January 2003 Proceedings of the First Asia-Pacific bioinformatics conference on Bioinformatics

Full text available:  pdf(6.40 MB)

Additional Information: full citation, abstract, reference

This paper describes knowledge-based homology modeling studies of envelope glycoprotein of Japanese encephalitis virus (JEVS). JEVS is a mosquito-borne *Flavivirus*, which is a major structural antigen and is responsible for viral hemagglutination and neutralization. The amino acids from the extra cellular domain of Egp of JEVS has been predicted using Tickborne encephalitis virus as a template.

Keywords: Japanese encephalitis virus, antigenic determinant, conformational epitope, homology modeling, loop modeling, molecular dynamics simulations, mutations, peptide vaccine, protein structure, property, three-dimensional structure

60 Large a polynomial-time nuclear vector replacement algorithm for automating NMR structural biology

Christopher James Langmead, Anthony Yan, Ryan Lilien, Lincong Wang, Bruce R. Ragan

April 2003 Proceedings of the seventh annual international conference on Computational Molecular Biology

Full text available:  pdf(2.14 MB)

Additional Information: full citation, abstract, references

High-throughput NMR structural biology can play an important role in structural biology. A new procedure for high-throughput NMR resonance assignment for a protein of known structure. These assignments are a prerequisite for probing protein-protein interactions and protein dynamics by NMR. Assignments are also the starting point for structure determination. This procedure is called *Nuclear Vector Replacement (NVR)* ...

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61 The side-chain positioning problem: a semidefinite programming formulatio

Bernard Chazelle, Carl Kingsford, Mona Singh

June 2003 Proceedings of the Paris C. Kanellakis memorial workshop on Principles o
Kanellakis memorial workshop on the occasion of his 50th birthday

Full text available: pdf(360.45 KB)

Additional Information: full citation, abstract, referen

Side-chain positioning is a central component of the protein structure prediction large body of research. The problem is NP-complete; in fact, it is even inapproximable. We investigate a variety of general search techniques and specialized heuristics. We investigate a semidefinite program. We introduce two novel rounding schemes and provide their effectiveness under various input ...

Keywords: protein side-chain positioning, randomized rounding, semidefinite programming

62 Lab report special section: information retrieval research in the University of

Peter Willett

December 1997

ACM SIGIR Forum, Volume 31 Issue 2

Full text available: pdf(644.64 KB)

Additional Information: full citation, index terms

63 The large scale parallelization of a conformational 3D Protein structure pre

Philip LoCascio, Kaizhi Yue, Peter Cummings, Ken Dill

November 1998

Proceedings of the 1998 ACM/IEEE conference on Supercomput

Full text available:  [html\(20.65 KB\)](#)

Additional Information: full citation, abstract

We present here the design strategy and performance analysis of a large scale s
3D Protein structures. The unique challenges which will be investigated are the
clock run time through the parallelization process, and the production of an appl
massively parallel configuration (currently 1024 nodes of the Intel Paragon) reli
supercomput ...



Keywords: massively parallel algorithm, protein folding

64 Efficient algorithms for local and global accessibility shading

Gavin Miller

July 1994

Proceedings of the 21st annual conference on Computer graphics and in

Full text available:  [pdf\(1.11 MB\)](#)  [ps\(13.03 MB\)](#)

Additional Information: full citation, abstract,

This paper discusses the use of two different approaches for computing the &ldc
These metrics characterize how easily a surface may be touched by a spherical
acceleration techniques for accessibility. The idea of surface accessibility is exte
accessibility” which measures the ability of a spherical probe to enter a s
locally on the surface. Th ...

Keywords: aging, surface accessibility shading, visualisation

65 Molecular applications of volume rendering and 3-D texture maps

David S. Goodsell, Arthur J. Olson

May 1989 Proceedings of the 1989 Chapel Hill workshop on Volume visualization

Full text available:  [pdf\(2.10 MB\)](#)

Additional Information: full citation, references, citings, index terms

Keywords: 3D texture map, ray-tracing, volume rendering

66 Spheres, molecules, and hidden surface removal

Dan Halperin, Mark H. Overmars

June 1994

Proceedings of the tenth annual symposium on Computational geometry

Full text available:  pdf(1.21 MB)

Additional Information: full citation, abstract, references, citations

We devise techniques to manipulate a collection of loosely interpenetrating spheres. This is motivated by the representation and manipulation of molecular configurations. We analyze the sphere model and point to its favorable properties that make it more suitable for a collection of spheres. For this special sphere model we present efficient algorithms for hidden surface removal.

67 Algorithmic issues in modeling motion

Pankaj K. Agarwal, Leonidas J. Guibas, Herbert Edelsbrunner, Jeff Erickson, Michael Hershberger, Christian Jensen, Lydia Kavraki, Patrice Koehl, Ming Lin, Dinesh Manolopoulos, David Mount, S. Muthukrishnan, Dinesh Pai, Elisha Sacks, Jack Snoeyink, Subhash Suri
December 2002
ACM Computing Surveys (CSUR), Volume 34 Issue 4

Full text available:  pdf(205.25 KB)

Additional Information: full citation, abstract, references, citations

This article is a survey of research areas in which motion plays a pivotal role. The article surveys approaches to modeling motion together with related data structures and algorithms that lie ahead in producing a more unified theory of motion representation that can be used in a wide variety of applications.

Keywords: Computational geometry, computer vision, mobile networks, modeling, physical simulation, robotics, spatio-temporal databases

68 Algorithmic strategies in combinatorial chemistry

Deborah Goldman, Sorin Istrail, Giuseppe Lancia, Antonio Piccolboni, Brian Walenz
February 2000
Proceedings of the eleventh annual ACM-SIAM symposium on Discrete Mathematics

Full text available:  pdf(940.84 KB)

Additional Information: full citation, references, index terms

69 Reconstructing a three-dimensional model with arbitrary errors

Bonnie Berger, Jon Kleinberg, Tom Leighton

March 1999

Journal of the ACM (JACM), Volume 46 Issue 2

Full text available:  pdf(174.41 KB)

Additional Information: full citation, abstract, references, citations

A number of current technologies allow for the determination of interatomic distances in proteins and RNA. Thus, the reconstruction of a three-dimensional set of points from distances has become a task of basic importance in determining molecular structure. Distances obtained from techniques such as NMR are typically sparse and error-prone, greatly complicating the reconstruction. Many of these errors result from experimental noise.

Keywords: biomolecular structure, distance geometry, random sampling, random walks

70 Collision detection for deforming necklaces

Leonidas Guibas, An Nguyen, Daniel Russel, Li Zhang

June 2002 Proceedings of the eighteenth annual symposium on Computational geometry

Full text available:  pdf(571.15 KB)

Additional Information: full citation, abstract, references,

In this paper, we propose to study deformable necklaces --- flexible chains of balls that may intersect. Such objects can be used to model macro-molecules, muscles, or objects in the physical world. In this paper, we exploit this linearity to develop geometric structures that are useful in physical simulations. We show how these structures can be implemented for necklace deformation ...

Keywords: bounding volume hierarchy, collision detection, deformable chains, p

71 Fast methods for simulation of biomolecule electrostatics

Shihhsien S. Kuo, Michael D. Altman, Jaydeep P. Bardhan, Bruce Tidor, Jacob K. W

November 2002 Proceedings of the 2002 IEEE/ACM international conference on Computational biology and bioinformatics

Full text available:  pdf(338.15 KB)

Additional Information: full citation, abstract, references,

Computer simulation is an important tool for improving our understanding of biomolecular systems in drug design. However, the numerical techniques used in these simulation tools are not widely used in analyzing integrated circuit interconnects. In this paper we describe a method to analyze biomolecule electrostatics, present an integral formulation of the problem, and a method to accelerate the solution ...

72 A self-consistent field optimization approach to build energetically and geometrically accurate protein models

Boris A. Reva, Alexei V. Finkelstein, Jeffrey Skolnick

March 1998 Proceedings of the second annual international conference on Computational molecular biology



Full text available:  pdf(532.94 KB)

Additional Information: full citation, references, index

73 I/O limitations in parallel molecular dynamics

Terry W. Clark, L. Ridgway Scott, Stanislaw Wlodek, J. Andrew McCammon

December 1995 Proceedings of the 1995 ACM/IEEE conference on Supercomputing (Supercomputing 1995)

Full text available:  pdf(183.44 KB)  html(2.39 KB)

Additional Information: full citation, references, index

74 A hierarchical load-balancing framework for dynamic multithreaded comput

Vijay Karamcheti, Andrew A. Chien

November 1998

Proceedings of the 1998 ACM/IEEE conference on Supercomputing

Full text available:  pdf(120.01 KB)

Additional Information: full citation, abstract

High-level parallel programming models that support dynamic fine-grained threads are increasingly popular for expressing irregular applications based on sophisticated data structures. However, implementing these multithreaded computations on such systems presents challenges, particularly with respect to load-balancing. Load-balancing techniques must be developed to support fine-grained parallelism with low overhead to support fine-grained parallelism.

75 On the complexity of protein folding (extended abstract)

Pierluigi Crescenzi, Deborah Goldman, Christos Papadimitriou, Antonio Piccolboni, et al.

May 1998

Proceedings of the thirtieth annual ACM symposium on Theory of computing

Full text available:  pdf(748.15 KB)

Additional Information: full citation, references, citations, index terms

76 On design principles for a molecular computer

Michael Conrad

May 1985

Communications of the ACM, Volume 28 Issue 5

Full text available:  pdf(2.50 MB)

Additional Information: full citation, abstract, references, citations, index terms

If the unique information-processing capabilities of protein enzymes could be adapted to design more efficient systems for such applications as pattern recognition and process control, the potential for a new class of molecular computers is great.

77 Reconstructing a three-dimensional model with arbitrary errors

Bonnie Berger, Jon Kleinberg, Tom Leighton

July 1996

Proceedings of the twenty-eighth annual ACM symposium on Theory of computing

Full text available:  pdf(1.18 MB)

Additional Information: full citation, references, index terms

78 Molecular docking using genetic algorithms

Yong L. Xiao, Donald E. Williams

April 1994

Proceedings of the 1994 ACM symposium on Applied computing

Full text available:  pdf(573.43 KB)

Additional Information: full citation, references, index terms

Keywords: function optimization, genetic algorithms, intermolecular interactions, molecular docking, protein-ligand interactions

79 Incorporating bioinformatics in an algorithms course

Lawrence D'Antonio

June 2003 ACM SIGCSE Bulletin , Proceedings of the 8th annual conference on Innovation in computer science education, Volume 35 Issue 3

Full text available:  pdf(342.73 KB)

Additional Information: full citation, abstract, references

In this paper we examine ways in which ideas from the exciting new field of bioinformatics can be incorporated into an algorithms course intended for computer science majors. Bioinformatics studies biological systems using the building blocks of life. Algorithms that involve searching, matching, or combinatorics are common in bioinformatics. These algorithms use many key ideas that are important to the field of computer programming. In addition, the algorithms often involve dynamic programming, which is a technique for solving complex problems by breaking them down into simpler subproblems. This paper discusses the challenges of teaching bioinformatics to computer science students and presents a course that integrates the two fields.

Keywords: bioinformatics, dynamic programming, palindromes, sequence alignment, common superstring problem

80 Special issue on on inductive logic programming: Ilp: a short look back and

David Page, Ashwin Srinivasan

December 2003

The Journal of Machine Learning Research, Volume 4

Full text available:  pdf(103.21 KB)

Additional Information: full citation, abstract, references

Inductive logic programming (ILP) is built on a foundation laid by research in machine learning. Armed with this strong foundation, ILP has been applied to important and interesting problems in engineering and the arts. This paper begins by briefly reviewing some examples of the benefits of ILP. In turn, the applications have brought into focus the need for more research in ILP. This paper discusses the challenges of teaching ILP to computer science students and presents a course that integrates the two fields.

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| 4 | 5,776,763 T Analytical process to determine biodegradability of chelants containing a double carboxy containing moiety |
| 5 | 5,616,497 T Method of chelating a metal ion to form a chelate and biodegrading the chelate |
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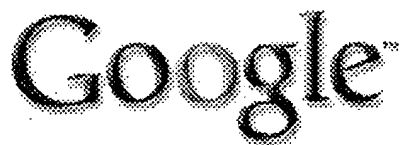
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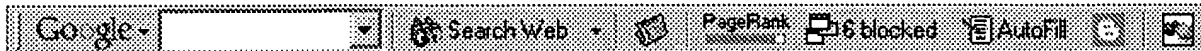
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3. [Protein Science -- Kerwin et al. 11 \(7\): 1825](#) 

... which only the carbon **atoms** CE3, CZ3, CH2, and CE2 ... lifetime caused by heavy-**atoms** species, like I-, relegated to ... static distribution of Trp-107-iodide **distances**. The accessibility of ...

www.proteinscience.org/cgi/content/full/11/7/1825

4. [Biophysical Journal -- Kostov and Freed 76 \(1\): 149](#) 

... tens of thousands of **atoms** and become prohibitively expensive ... friction coefficients for **atoms** or groups of **atoms** in the polymer ... However, plots of interatomic **distances** as a function of ...

www.biophysj.org/cgi/content/full/76/1/149

5. [Nucl. Acids. Res. -- Boutselakis et al. 31 \(1\): 458](#) 

... into residues and finally the constituent **atoms**. Derived data are ... In addition, the actual **distances**, angles and the angles ... the database associates the **atoms** with energy types from ...

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6. [E-MSD: the European Bioinformatics Institute Macromolecular Structure Database \(PDF\)](#) 

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7. <http://www.omg.org/docs/lifesci/00-02-08.idl> 

... The number of hydrogen **atoms** attached to the atom at ... site // excluding any H **atoms** for which coordinates (measured or ... identifies a cluster of **atoms** that show long range // positional ...

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8. [99.05.02: The Amazing Dna Molecule: Its History, Structure and Function](#) 

... of regularly spaced **atoms** that exist in a ... contain **atoms** that are separated from each other by **distances** that are ... to detect these **distances** since their

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9. [Meeting Abstracts](#)

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carbon **atoms** are shown in ... Table 2. Interaction **distances** in the complex of ...

www.pnas.org/cgi/content/full/95/22/12956

11. [ANU - RSPHYSSE Annual Report 1998](#)

Director's Report. 7 Statistics. Applied Mathematics. Research Summary ... colloidal:

the behaviour of **atoms** or molecules, or complex mixtures ... in a range of

distances after the polymer molecules become ... of interaction between two **atoms**

is correct only in the ...

www.rsphysse.anu.edu.au/admin/AR98/am.html

12. [Glossary of biotechnology for food and agriculture](#)

A Abbreviation for adenine. Ab Abbreviation for antibody. ABC model Widely

accepted model of flower organ identity that appears generally applicable to distantly

related dicotyledonous, although less well to monocotyledonous plants.

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... Higesolution Photoelectron Spectroscopy in **Atoms** and Molecules ... CG5 Rost,

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orgs.unt.edu/CAARI/PROGRAMABSTRACT.html

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